1,3-Dioxolane 646-06-0 | DTXSID4027284

M	odel	Performance	١
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Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 80.6 °C

Global applicability domain: Inside

Local applicability domain index: 6.90e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dioxolane Measured: 78.0 Predicted: 80.6 Image not found

Methyl chlorocarbonate

Measured: 70.5 **Predicted:** 71.7

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Butyraldehyde Measured: 74.8 Predicted: 71.3

Image not found

Methyl ethyl ketone Measured: 79.5 Predicted: 72.4 Image not found

Epichlorohydrin Measured: 117 Predicted: 103 Image not found

Epichlorohydrin Measured: 117 Predicted: 103